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14. ABSTRACT

In this project we aim to construct a high fidelity boundary condition module for Maxwell's equations that can be interfaced with major time-domain electromagnetics solver systems. There is ample need in the EM modeling community for reliable and stable far field boundary conditions of high accuracy. Most existing methods are limited in one or more of these requirements, and recent developments in the CRBC procedure (as originally presented by Hagstrom and Warburton in 2009), have made the technique an attractive candidate for implementation in multi-purpose solvers. In phase-I of this project

15. SUBJECT TERMS

computational electromagnetics, time domain, high order accuracy, outer boundary condition, modular software

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Cover Page

Contract Number:	**W911NF-13-C-0039**
Proposal Number:	**A2-5030**
Contractor's Name and Address:	HyPerComp, Inc. 2629 Townsgate Road, Suite 105 Westlake Village, CA 91361
Title of the Project:	**A Priori Error-Controlled Simulation of Electromagnetic Phenomena for HPC**
Contract Performance Period:	March 13, 2013 - March 12, 2015
Current Reporting Period:	June 13, 2013 - September 12, 2013

Total Contract Amount:	$749,996
Amount of funds paid by DFAS to date:	$151,169
Total amount expended/invoiced to date:	$160,505
Number of employees working on the project:	3
Number of new employees placed on contract this month:	0

Contents

1 Abstract

In this project we aim to construct a high fidelity boundary condition module for Maxwell's equations that can be interfaced with major time-domain electromagnetics solver systems. There is ample need in the EM modeling community for reliable and stable far field boundary conditions of high accuracy. Most existing methods are limited in one or more of these requirements, and recent developments in the CRBC procedure (as originally presented by Hagstrom and Warburton in 2009), have made the technique an attractive candidate for implementation in multi-purpose solvers. In phase-I of this project we implemented and improved upon many aspects of this method, particularly in light of the needs of high order accurate Maxwell equations solvers (based on the discontinuous Galerkin method). Error bounds were computed and demonstrated for a number of cases. We continue in the second phase of this project to improve upon the robustness of this method, as we develop a software platform which shall be its flagship (and open source) implementation. In this second quarterly report we present a novel way to construct a upwinding numerical flux which solves the remaining problem from phase I of the project - instability issues of CRBC coupling with DG solver in 2D.

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2 Introduction

In this project, HyPerComp is collaborating with Prof. Thomas Hagstrom and his research group at the Southern Methodist University (SMU). Roles of the two organizations are very broadly divided into mathematical method development (led by SMU) and implementation, software development and maturation (led by HyPerComp). The project is coordinated via a series of in-person and telephone meetings. We have been conducting weekly telephone meetings. Two students, John Lagrone and Fritz Juhnke have been included in the team and have been actively participating in the work so far.

Tasks: The following is a list of tasks to be performed in this project.

1. Project Formulation
2. Software Development
3. Verification & Validation
4. Coupling
5. Efficiency Testing
6. Release of software
7. Documentation
8. Sustainability Plan
9. User Support

At present, we are working on solving the remaining instability problem from phase I and testing it in sample problems. Primary concerns pertaining to method stability at corners, particularly in 3D are being addressed. CRBC implementations in finite difference schemes, DG (in FORTRAN as well as in MATLAB) are available from prior research in this project, for testing.

We are presently aiming to integrate the CRBC module with the following codes:

- HDphysics from HyPerComp, a high order DG based solver
- MEEP from MIT, an open source FDTD code
- cgmx part of "Overture" suite of simulation codes from LLNL - high order finite differences, second order PDEs
- CLAWPACK a finite difference suite of solvers from U.Washington

Students from SMU focus on an FDTD implementation of CRBC in the Yee scheme for a 3D waveguide. Thomas Hagstrom starts to fomulate the CRBC for Maxwell's equation in 3+1-Dimensions include edges and corners. We are in the process of developing software requirements for each of the systems mentioned above, so that we can outline a common implementation of the method and programming techniques. We will also begin to implement prototype of CRBC with DG for Maxwell's equation in 3D. These shall be discussed in the forthcoming report.

3 Instability issue solved - upwinding flux on CRBC

In phase I of the project, we have experienced some instability issue with the CRBC coupling with DG when $N_{bc} = 3$ and $N_{dg} \geq 10$ on unstructured meshes (We have never encountered any stability issus on the structured mesh). Since we didn't know what is an appropriate upwinding numerical flux to use, we simply choosed central flux for CRBC. This choice turns out to be instable even after we reformulate the CRBC on the corner and forbid to split the element adjacent to the corner (See next section for more details of the recap of the instability issue). After more comprehensive tests and debug, we have found that unbalanced numerical flux between volume (upwinding flux) and CRBC boundary (central flux) caused the instability, since there isn't enough dissipation for the CRBC. Now with the new Maxwell like upwinding numerical flux term, we are able to solve the instability issue. A rigorous proof of the stability have not been achieved yet. However, we haven't experienced any instability issue in numerous testing problems with varying N_{bc}, N_{dg}, dt (See next section). Details of mathematical definitions of the numerical flux terms are described below.

Consider the TM Maxwell system:

$$\begin{aligned} \frac{\partial H^x}{\partial t} + \frac{1}{\mu}\frac{\partial E^z}{\partial y} &= 0 \qquad (1)\\ \frac{\partial H^y}{\partial t} - \frac{1}{\mu}\frac{\partial E^z}{\partial x} &= 0 \qquad (2)\\ \frac{\partial E^z}{\partial t} - \frac{1}{\epsilon}\frac{\partial H^y}{\partial x} + \frac{1}{\epsilon}\frac{\partial H^x}{\partial y} &= 0 \qquad (3)\end{aligned}$$

and set $c = \frac{1}{\sqrt{\epsilon\mu}}$. Consider a portion of the radiation boundary with unit normal n pointing outward from the computational domain and unit tangent vector τ:

$$n = \begin{pmatrix} n_x \\ n_y \end{pmatrix}, \quad \tau = \begin{pmatrix} -n_y \\ n_x \end{pmatrix}. \qquad (4)$$

$$R_{\pm,j} = E^z_j \pm \sqrt{\frac{\mu}{\epsilon}}\left(-n_y H^x_j + n_x H^y_j\right), \quad H_{n,j} = n_x H^x_j + n_y H^y_j, \qquad (5)$$

From the CRBC iteration of TM Maxwell equation, we are solving a 1d system of PDEs along the boundary.

$$\begin{aligned} &(1-\cos\phi_j)\frac{\partial}{\partial t}R_{-,j-1} - \frac{1}{T}\frac{\sin^2\phi_j}{\cos\phi_j}R_{-,j-1} + \frac{1}{\epsilon}\frac{\partial}{\partial\tau}H_{n,j-1} = \qquad (6)\\ &(1+\cos\bar{\phi}_j)\frac{\partial}{\partial t}R_{-,j} + \frac{1}{T}\frac{\sin^2\bar{\phi}_j}{\cos\bar{\phi}_j}R_{-,j} + \frac{1}{\epsilon}\frac{\partial}{\partial\tau}H_{n,j}.\end{aligned}$$

$$\begin{aligned} &(1+\cos\phi_j)\frac{\partial}{\partial t}R_{+,j-1} + \frac{1}{T}\frac{\sin^2\phi_j}{\cos\phi_j}R_{+,j-1} + \frac{1}{\epsilon}\frac{\partial}{\partial\tau}H_{n,j-1} = \qquad (7)\\ &(1-\cos\bar{\phi}_j)\frac{\partial}{\partial t}R_{+,j} - \frac{1}{T}\frac{\sin^2\bar{\phi}_j}{\cos\bar{\phi}_j}R_{+,j} + \frac{1}{\epsilon}\frac{\partial}{\partial\tau}H_{n,j}.\end{aligned}$$

$$\frac{\partial}{\partial t}H_{n,j} + \frac{1}{2\mu}\frac{\partial}{\partial\tau}(R_{+,j} + R_{-,j}) = 0 \qquad (8)$$

This yields the local semidiscrete scheme equation (9), (10), (11)

$$\begin{aligned}\frac{\partial}{\partial t}R_{-,j} = \frac{1}{(1+\cos\bar{\phi}_j)}\{&(1-\cos\phi_j)\frac{\partial}{\partial t}R_{-,j-1}\\ &-\frac{1}{T}\frac{\sin^2\bar{\phi}_j}{\cos\bar{\phi}_j}R_{-,j}-\frac{1}{T}\frac{\sin^2\phi_j}{\cos\phi_j}R_{-,j-1}\\ &+\frac{1}{\epsilon}[D_\tau(H_{n,j-1}-H_{n,j})+\frac{1}{2}(JM)^{-1}\oint_{x_l}^{x_r} n\cdot(f_1-f_1^*)l(x)dx]\}\end{aligned} \tag{9}$$

$$\begin{aligned}\frac{\partial}{\partial t}R_{+,j-1} = \frac{1}{(1+\cos\phi_j)}\{&(1-\cos\bar{\phi}_j)\frac{\partial}{\partial t}R_{+,j}\\ &-\frac{1}{T}\frac{\sin^2\bar{\phi}_j}{\cos\bar{\phi}_j}R_{+,j}-\frac{1}{T}\frac{\sin^2\phi_j}{\cos\phi_j}R_{+,j-1}\\ &+\frac{1}{\epsilon}[D_\tau(H_{n,j}-H_{n,j-1})+\frac{1}{2}(JM)^{-1}\oint_{x_l}^{x_r} n\cdot(f_2-f_2^*)l(x)dx]\}\end{aligned} \tag{10}$$

$$\frac{\partial}{\partial t}H_{n,j} = -\frac{1}{2\mu}\{D_\tau(R_{+,j}+R_{-,j})+\frac{1}{2}(JM)^{-1}\oint_{x_l}^{x_r} n\cdot(f_3-f_3^*)l(x)dx\} \tag{11}$$

The numerical flux for each iteration are

$$\begin{aligned}n\cdot(f_1-f_1^*) &= n\cdot([[H_{n,j}]]-[[H_{n,j-1}]])\\ &\quad -\frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}([[R_{-,j}]]-[[R_{-,j-1}]]+[[R_{+,j}]]-[[R_{+,j-1}]])\end{aligned} \tag{12}$$

$$\begin{aligned}n\cdot(f_2-f_2^*) &= n\cdot([[H_{n,j-1}]]-[[H_{n,j}]])\\ &\quad +\frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}([[R_{-,j}]]-[[R_{-,j-1}]]+[[R_{+,j}]]-[[R_{+,j-1}]])\end{aligned} \tag{13}$$

$$n\cdot(f_3-f_3^*) = n\cdot([[R_{+,j}]]+[[R_{-,j}]])-\sqrt{\frac{\epsilon}{\mu}}[[H_{n,j}]] \tag{14}$$

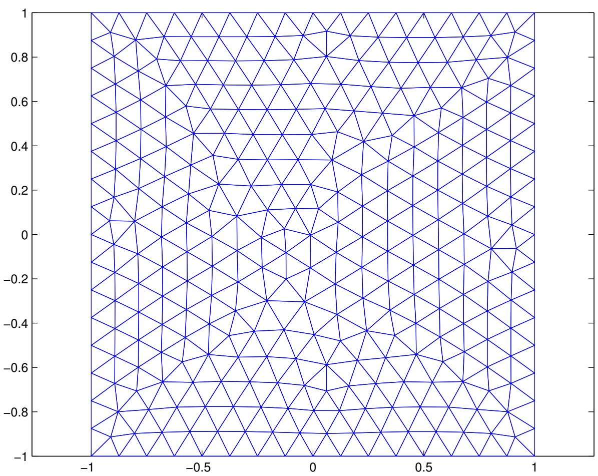
$[[q]] = q^- - q^+$, $n = -1, 1$ depending on the direction since we are solving a 1d system of PDEs. Note that we are solving $R_{-,j}$ in an increasing order and $R_{+,j}$ in a decreasing order.

4 Numerical validation

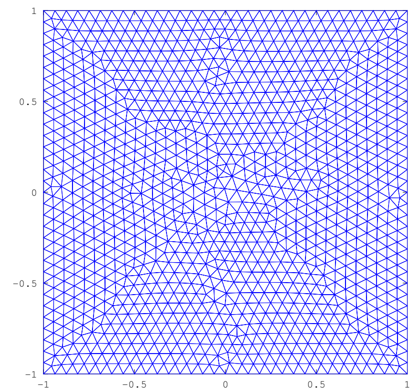
4.1 Recap of Instability issue in phase I

The original implementation of CRBC (using central flux) coupling with DG on a unstructured grid is not completely stable, especially for some combination of DG order N_{dg}, CRBC order N_{bc} and timestep size dt (for example, $N_{dg} = 10$, $N_{bc} = 3$). After many tests on different grids (see figures 1, 2 (a)(b)) with different topology, grid size, domain and time step size, we confirm that it will become unstable eventually. The fix in phase I by enforcing only one element along the corner is not sufficient. The only major difference between mesh figures 1 (c) and (d) are at the corners, and in both cases the solution start to blow out around time $T = 15$ with $Finaltime = 100$. From figure 3, 4 (little white triangular sharped noise along the boundary), we can see that instability starts between the CRBC boundary elements and accumulates along the boundaries, which is independent of whether or not the corners have been cutted, nor the size of the domain. With default timestep size setting, $N_{dg} = 10$ and $N_{bc} \leq 3$, in every case the solution starts to blow up around time $T = 10$, $Finaltime = 100$, except for grid squarecartnx50(see figure 1(e)) when all the triangular elements are obtained by splitting the square elements. However, this still become unstable when much smaller timestep is used (see figure 5, $dt = 1.25e - 3$ is default timestep size).

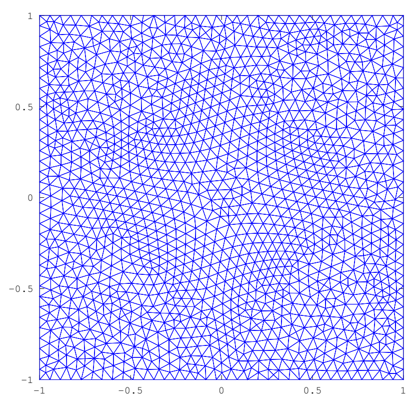
The reason is that there is not enough dissipation to keep the method stable when central flux is used along CRBC. The upwinding numerical flux we used on volume integration to keep the method stable does not provide enough dissipation for the CRBC to be stable. And there is no dissipation coming from the boundary since only central flux is used on CRBC. The smaller timestep size is, the less dissipative the method becomes. From figure 6, it is more obvious to see how different timestep size affect the dissipation of the original algorithm. The instability is not very strong and vanishes when N_{bc} is big even if the central flux is used on CRBC. Empirically, when $N_{bc} = 3$, provide enough dissipation for the method to be stable with $N_{dg} \leq 5$, and when $N_{bc} \geq 4$, it provide enough dissipation for at least $N_{dg} = 10$. Practically speaking, even if we use central flux on CRBC, when N_{bc} is big, we usually don't see any instability, but smaller timestep size will reduce the stability of CRBC.



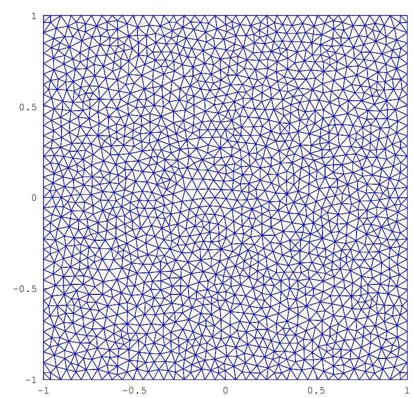
(a) 0125



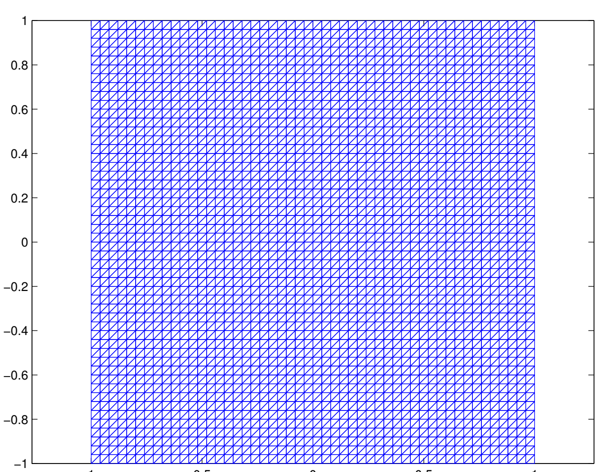
(b) 00625



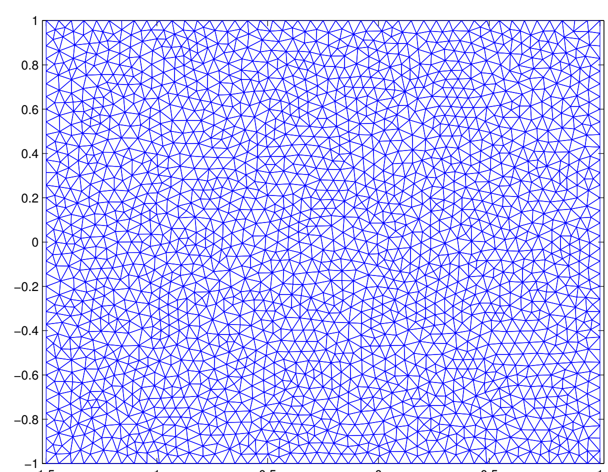
(c) free4



(d) free4goodcorner

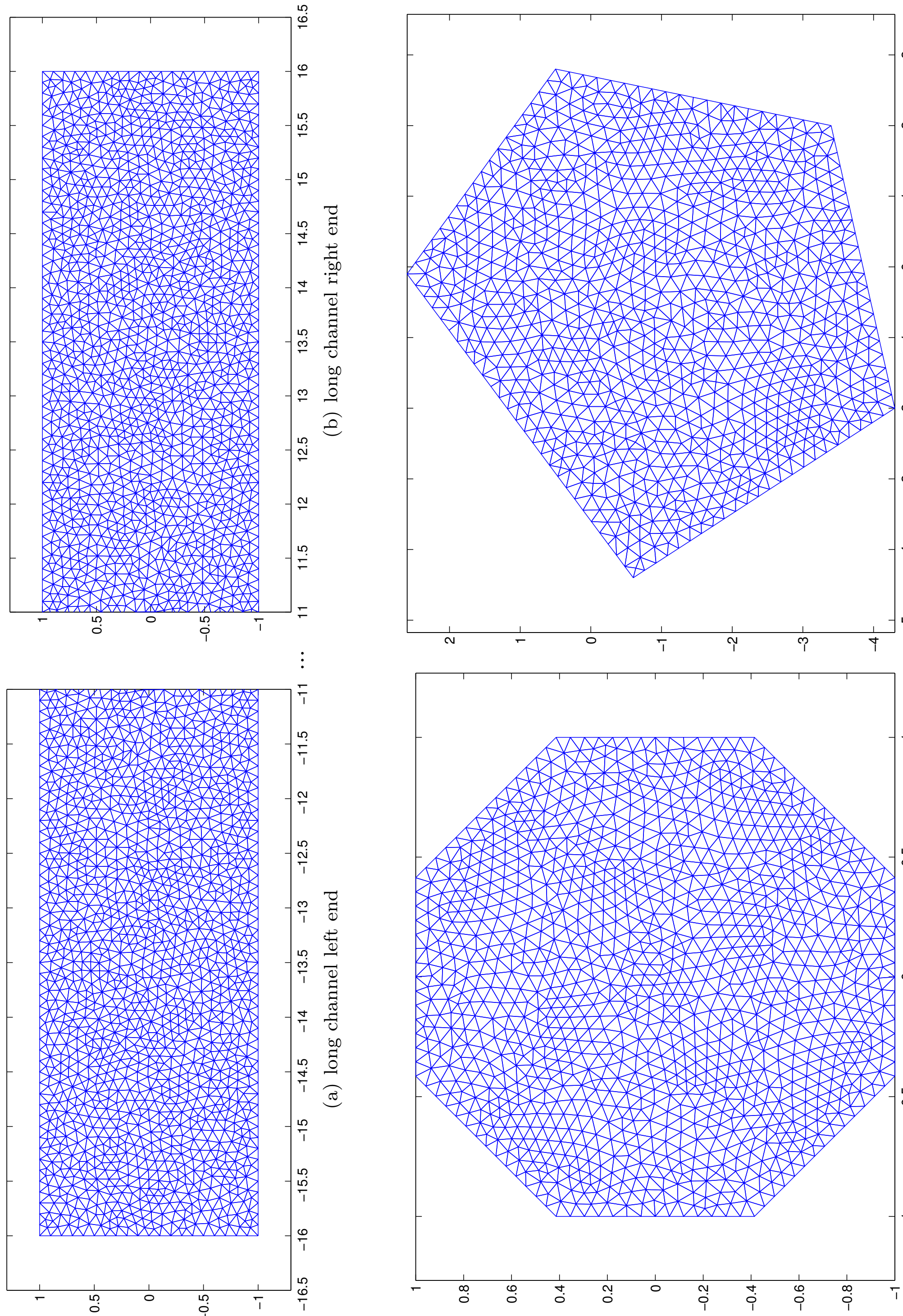


(e) squarecartnx50



(f) free4wide

Figure 1: List of the meshs part I.



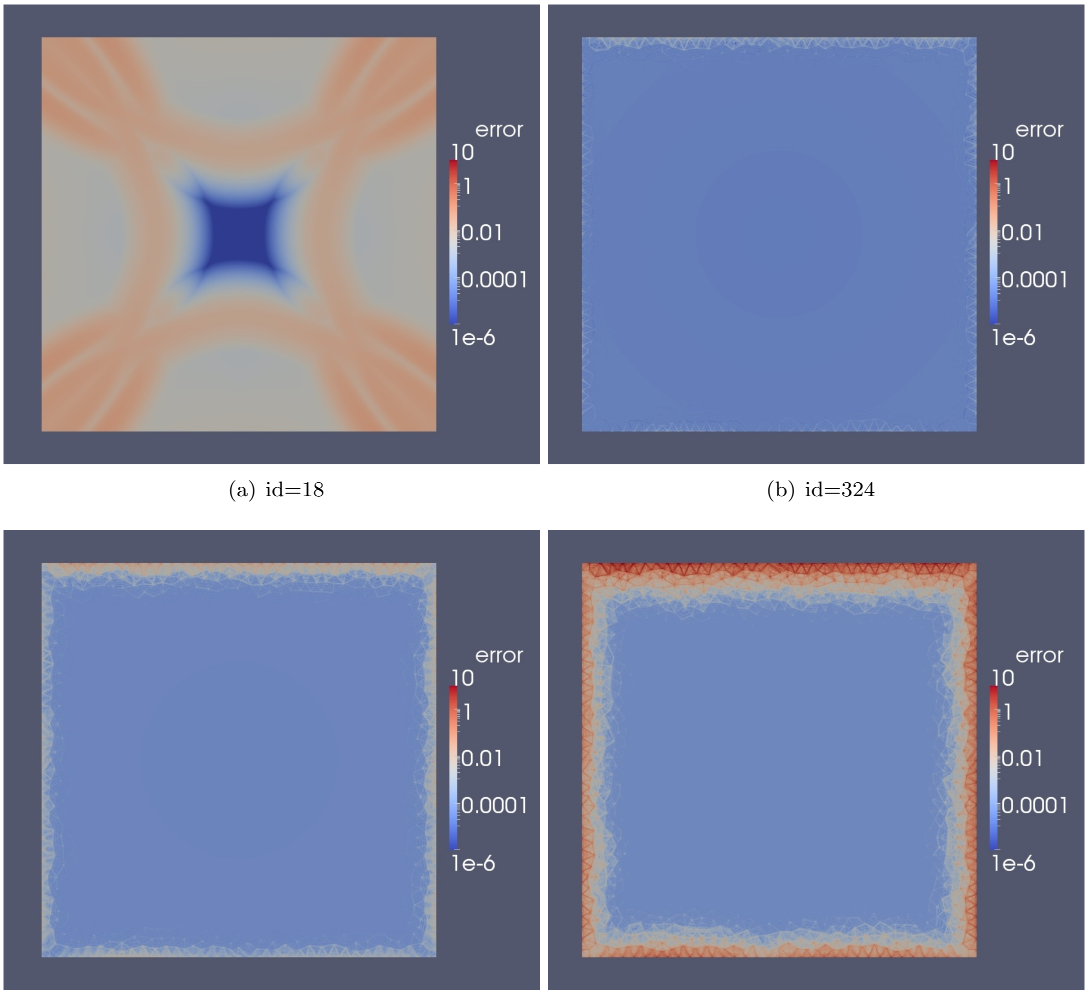
(a) long channel left end

(b) long channel right end

(c) freeregoct2

(d) handdraw

Figure 2: List of the meshs part II.



(a) id=18

(b) id=324

(c) id=364

(d) id=424

Figure 3: Snapshot of the instability along the boundary at 4 different time for grid free4goodcorner(see figure 1(d)) using old flux term.

(a) id=137

(b) id=207

(c) id=247

(d) id=287

Figure 4: Snapshot of the instability along the boundary at 4 different time for grid longchannel(see figure 2(a), 2(b)) using old flux term.

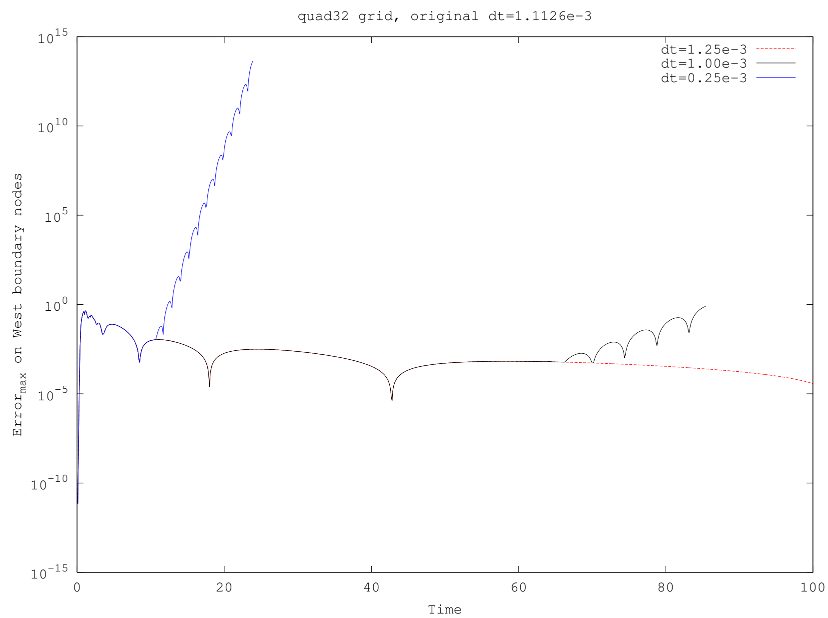


Figure 5: Error on the boundary nodes for grid quad32(see figure 1(e)) with different timestep size using old flux term.

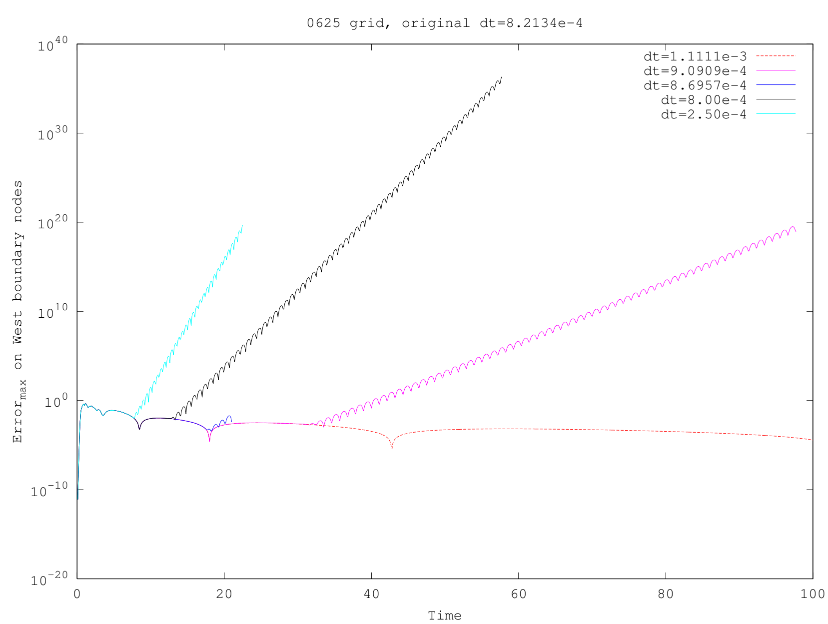


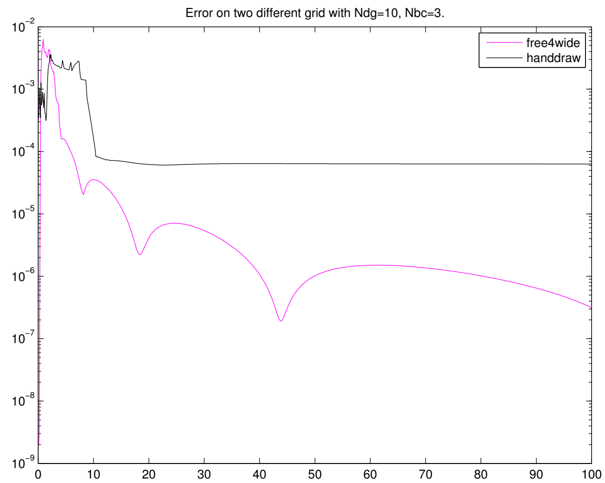
Figure 6: Error on the boundary nodes for grid 00625(see figure 1(b)) with different timestep size using old flux term.

4.2 Unconditionally stable with upwinding numerical flux in 2D

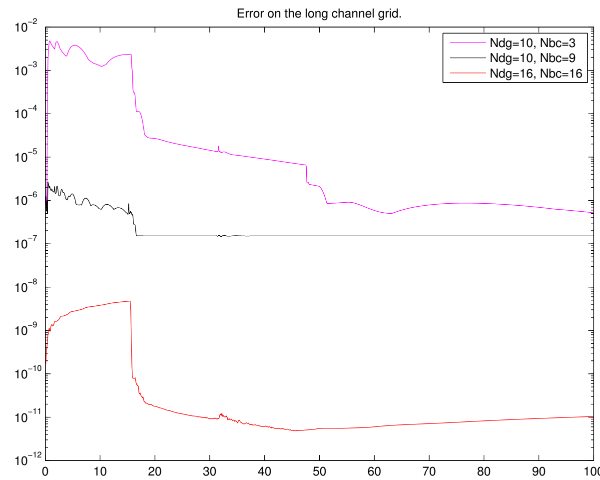
The instability issue is completely solved in our new implementation of the CRBC with new upwinding numerical flux along the CRBC boundary as described in last section. We have tested the new method on all meshes (see figure 1, 2) with various mesh size, topology, geometry, computational domain, time step size dt, DG order DG N_{dg}, CRBC order N_{bc}, and they are all stable upto time finaltime $T = 100$. Details of numerical experiments are summarized in table 4.2. Error results along time are shown in 7, which clearly shows great advantage over our old implementation of CRBC for TM Maxwell's equation in 2D.

gridname	Ndg	Nbc	K	orig. dt	running dt	Note
0125	20	3	568	5.36E-004	1.00E-004	square shape
00625	10	3	2310	8.21E-004	1.00E-004	
00625	10	3	2310	8.21E-004	5.00E-004	
square_cart_nx50	10	3	5000	7.12E-004	5.00E-004	
free4	10	3	2890	6.93E-004	1.00E-004	
free4	10	3	2890	6.93E-004	5.00E-004	
free4_goodcorner	10	3	3198	6.00E-004	5.00E-004	
free_regoct_2	15	3	2210	3.57E-004	2.50E-004	octagon
	10	3		7.26E-004	5.00E-004	
	10	5		7.26E-004	5.00E-004	
	10	9		7.26E-004	5.00E-004	
	8	5		1.10E-003	5.00E-004	
	8	9		1.10E-003	5.00E-004	
long_channel	10	3	16658	1.10E-003	5.00E-004	long channel
	10	9		1.10E-003	5.00E-004	
	16	16		4.67E-004	4.55E-004	
handdraw	10	3	1823	2.30E-004	2.00E-003	arbitrary polygon
free_4_wide	10	3	4048	6.27E-004	5.00E-004	rectangle

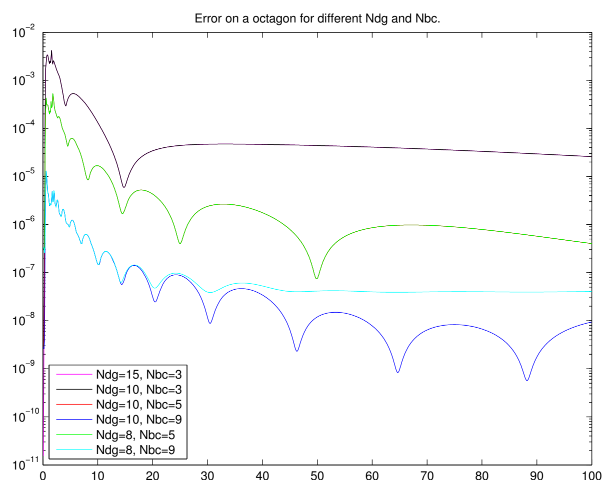
Table 1: CRBC with new flux term experiments summary.



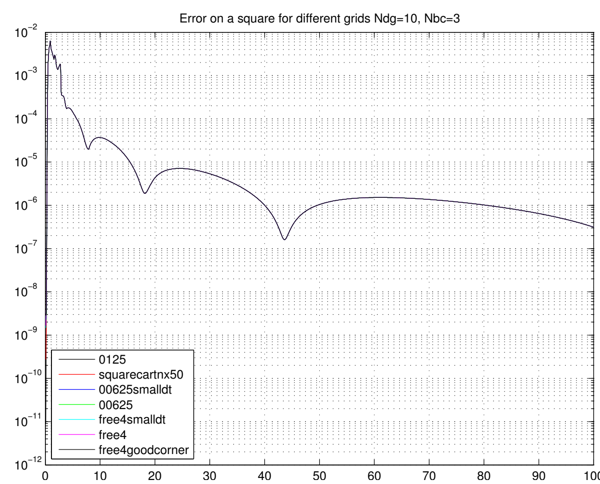
(a) Error for handdraw polygon and a rectangle.



(b) Error for 32 by 2 long channel.



(c) Error for an octagon, two cases of Nbc=3 and Nbc=5 overlaps.



(d) Error on a unit square, everything overlaps.

Figure 7: Error plot for various meshes and parameters using new flux term in CRBC.